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1 Melléklet
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3 A 2025. évi OTDK dolgozatomhoz használt reakciómechanizmus, amely tartalmazza a
4 reakciók Arrhenius-paramétereit, a harmadiktest-reakciók harmadiktest-együtthatóit,
5 a nyomásfüggő reakciók alsó nyomáshatárra vonatkozó Arrhenius-konstansait, a Troe-
6 típusú
7 nyomásfüggő reakciók Troe-paramétereit, a PLOG-reakciók paramétereit, és az egyes
8 anyagok NASA-paramétereit.
9
10 ELEMENTS
11 AR C H HE N !!O
12 END
13
14 SPECIES
15 AR H H2 H2NN !!H2NO H2O H2O2
16 HE
17 !!HNO HNO2 HNOH HO2 HON HONO HONO2
18 N N2 N2H2 N2H3
19 N2H4 !!N2O
20 NH NH2
21 !!NH2OH
22 NH3 NNH !!NO NO2 NO3 O O2 OH
23 END
24
25 THERMO ALL
26 300.0000 1000.00 5000.0000
27 ! Refitting species AR:
28 ! max difference Cp/R = 2.6645e-15 at T = 556.2781 K
29 ! max difference H/RT = 1.5543e-15 at T = 1003.0015 K
30 ! max difference S/R = 7.1054e-15 at T = 398.7494 K
31 ! T_match = 1000.000000 jump
32 ! Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 0.000e+00, 0.000e+00)
33 AR AR 1 0 0 OG 300.0000 5000.0000 1000.00 1
34 2.50000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
35 -7.45375000e+02 4.36600000e+00 2.50000000e+00 -1.56525602e-16 4.56943616e-19 3
36 -5.17814989e-22 1.99020834e-25 -7.45375000e+02 4.36600000e+00 4
37 ! Refitting species H:
38 ! max difference Cp/R = 1.2446e-09 at T = 998.9995 K
39 ! max difference H/RT = 2.8133e-09 at T = 1000.6503 K
40 ! max difference S/R = 8.5018e-09 at T = 1000.6503 K
41 ! T_match = 1000.000000 jump
42 ! Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 0.000e+00, 0.000e+00)
43 H H 1 0 0 OG 200.0000 3500.0000 1000.00 1
44 2.50000001e+00 -2.30842973e-11 1.61561948e-14 -4.73515235e-18 4.98197357e-22 2
45 2.54736599e+04 -4.46682905e-01 2.50000000e+00 -3.88870807e-11 1.07986092e-13 3
46 -1.20667212e-16 4.54829892e-20 2.54736599e+04 -4.46682873e-01 4
47 ! Refitting species H2:
48 ! max difference Cp/R = 2.5860e-02 at T = 200.0000 K
49 ! max difference H/RT = 4.7055e-03 at T = 200.0000 K
50 ! max difference S/R = 4.1717e-03 at T = 200.0000 K
51 ! T_match = 1000.000000 jump
52 ! Delta(Cp/R, H/RT, S/R) = (-4.441e-16, 0.000e+00, 0.000e+00)
53 H2 H 2 0 0 OG 200.0000 3500.0000 1000.00 1
54 3.33727920e+00 -4.94024731e-05 4.99456778e-07 -1.79566394e-10 2.00255376e-14 2
55 -9.52851692e+02 -3.20685584e+00 2.63703014e+00 5.51055679e-03 -1.21759447e-05 3
56 1.12923549e-08 -3.63620454e-12 -9.44182766e+02 -5.01881510e-01 4
57 ! Refitting species H2NN:
58 ! max difference Cp/R = 4.0712e-02 at T = 200.0000 K
59 ! max difference H/RT = 7.4081e-03 at T = 200.0000 K
60 ! max difference S/R = 6.5678e-03 at T = 200.0000 K
61 ! T_match = 1000.000000 jump
62 ! Delta(Cp/R, H/RT, S/R) = ( 1.776e-15, -7.105e-15, 0.000e+00)
63 H2NN H 2N 2 0 OG 200.0000 6000.0000 1000.00 1
64 3.05903670e+00 6.18382347e-03 -2.22171165e-06 3.58539206e-10 -2.14532905e-14 2
65 3.48572542e+04 6.70182016e+00 4.07123144e+00 -3.43561618e-03 1.85841969e-05 3
66 -1.64437379e-08 4.58216019e-12 3.49993230e+04 3.37616765e+00 4
67 ! Refitting species H2NO:
68 ! max difference Cp/R = 1.9886e-06 at T = 1499.3997 K
69 ! max difference H/RT = 4.7413e-07 at T = 1501.2506 K
70 ! max difference S/R = 8.3926e-06 at T = 1501.2506 K
71 ! T_match = 1500.000000 jump
72 ! Delta(Cp/R, H/RT, S/R) = ( 1.776e-15, 0.000e+00, 0.000e+00)
73 !!H2NO H 2O 1N 1 OG 300.0000 4000.0000 1500.00 1

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72 !! 5.67334600e+00 2.29883700e-03-1.77444600e-07-1.10348200e-10 1.85976200e-14 2
73 !! 5.56932571e+03-6.15353161e+00 2.53059296e+00 8.59601653e-03-5.47099406e-06 3
74 !! 2.27622271e-09-4.64801256e-13 6.86802967e+03 1.12664973e+01 4
75 ! Refitting species H2O:
76 ! max difference Cp/R = 1.7826e-04 at T = 200.0000 K
77 ! max difference H/RT = 3.2437e-05 at T = 200.0000 K
78 ! max difference S/R = 2.8758e-05 at T = 200.0000 K
79 ! T_match = 1000.000000 jump
80 ! Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 0.000e+00, 0.000e+00)
81 !!H2O H 20 1 0 OG 200.0000 3500.0000 1000.00 1
82 !! 3.03399249e+00 2.17691804e-03-1.64072518e-07-9.70419870e-11 1.68200992e-14 2
83 !!-3.00042785e+04 4.96678276e+00 4.19662285e+00-2.01940753e-03 6.47006475e-06 3
84 !!-5.42686127e-09 1.74619732e-12-3.02935458e+04-8.40864214e-01 4
85 ! Refitting species H2O2:
86 ! max difference Cp/R = 3.0404e-02 at T = 200.0000 K
87 ! max difference H/RT = 5.5324e-03 at T = 200.0000 K
88 ! max difference S/R = 4.9049e-03 at T = 200.0000 K
89 ! T_match = 1000.000000 jump
90 ! Delta(Cp/R, H/RT, S/R) = ( 3.553e-15, 0.000e+00, 0.000e+00)
91 !!H2O2 H 20 2 0 OG 200.0000 3500.0000 1000.00 1
92 !! 4.16500285e+00 4.90831694e-03-1.90139225e-06 3.71185986e-10-2.87908305e-14 2
93 !!-1.78586218e+04 2.91831124e+00 3.93197775e+00 2.36118766e-03 8.14814882e-06 3
94 !!-1.11544079e-08 4.22741638e-12-1.76717220e+04 4.82816319e+00 4
95 ! Refitting species HE:
96 ! max difference Cp/R = 1.7764e-15 at T = 200.0000 K
97 ! max difference H/RT = 8.8818e-16 at T = 208.7044 K
98 ! max difference S/R = 3.5527e-15 at T = 437.9190 K
99 ! T_match = 1000.000000 jump
100 ! Delta(Cp/R, H/RT, S/R) = ( 4.441e-16, 0.000e+00, 0.000e+00)
101 HE HE 1 0 0 OG 200.0000 6000.0000 1000.00 1
102 2.50000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
103 -7.45375000e+02 9.28723974e-01 2.50000000e+00-1.21434192e-16 3.14642268e-19 3
104 -3.30872200e-22 1.21191563e-25-7.45375000e+02 9.28723974e-01 4
105 ! Refitting species HNO:
106 ! max difference Cp/R = 5.4156e-07 at T = 946.5733 K
107 ! max difference H/RT = 2.9043e-06 at T = 1000.6503 K
108 ! max difference S/R = 2.5931e-06 at T = 1054.7274 K
109 ! T_match = 1000.000000 jump
110 ! Delta(Cp/R, H/RT, S/R) = ( 4.441e-15, 0.000e+00, 0.000e+00)
111 !!HNO H 10 1N 1 OG 300.0000 5000.0000 1000.00 1
112 !! 3.61514400e+00 3.21248600e-03-1.26033700e-06 2.26729800e-10-1.53623600e-14 2
113 !! 1.06619129e+04 4.81026141e+00 2.78439387e+00 6.60971610e-03-9.30040950e-06 3
114 !! 9.43818504e-09-3.75322506e-12 1.09187809e+04 9.03566675e+00 4
115 ! Refitting species HNO2:
116 ! max difference Cp/R = 1.8131e-06 at T = 1423.5118 K
117 ! max difference H/RT = 3.1425e-07 at T = 1499.3997 K
118 ! max difference S/R = 3.2152e-06 at T = 1501.2506 K
119 ! T_match = 1500.000000 jump
120 ! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 0.000e+00, 7.105e-15)
121 !!HNO2 H 10 2N 1 OG 300.0000 4000.0000 1500.00 1
122 !! 6.47963000e+00 1.99527400e-03-1.74038700e-07-9.69587200e-11 1.70148000e-14 2
123 !!-7.80950328e+03-1.06771486e+01 1.93482897e+00 1.01004186e-02-4.96473863e-06 3
124 !! 8.70212516e-10-2.35191805e-15-5.91571493e+03 1.47282468e+01 4
125 ! Refitting species HNOH:
126 ! max difference Cp/R = 5.1536e-02 at T = 200.0000 K
127 ! max difference H/RT = 9.3778e-03 at T = 200.0000 K
128 ! max difference S/R = 8.3140e-03 at T = 200.0000 K
129 ! T_match = 1000.000000 jump
130 ! Delta(Cp/R, H/RT, S/R) = ( 8.882e-16, 0.000e+00, 0.000e+00)
131 !!HNOH H 20 1N 1 OG 200.0000 6000.0000 1000.00 1
132 !! 3.98321933e+00 4.88846374e-03-1.65086637e-06 2.55371446e-10-1.48308561e-14 2
133 !! 1.05833771e+04 3.62948054e+00 3.37275545e+00 1.89634132e-03 1.11346941e-05 3
134 !!-1.38975267e-08 4.95509312e-12 1.09722885e+04 7.92090954e+00 4
135 ! Refitting species HO2:
136 ! max difference Cp/R = 3.2883e-02 at T = 200.0000 K
137 ! max difference H/RT = 5.9836e-03 at T = 200.0000 K
138 ! max difference S/R = 5.3048e-03 at T = 200.0000 K
139 ! T_match = 1000.000000 jump
140 ! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 0.000e+00, 0.000e+00)
141 !!HO2 H 10 2 0 OG 200.0000 3500.0000 1000.00 1
142 !! 4.01721090e+00 2.23982013e-03-6.33658150e-07 1.14246370e-10-1.07908535e-14 2
143 !! 1.15280867e+02 3.78743242e+00 3.92960049e+00-1.60830209e-03 1.18727670e-05 3
144 !!-1.30037956e-08 4.53655859e-12 3.28184607e+02 5.22337662e+00 4

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145 ! Refitting species HON:
146 !   max difference Cp/R = 8.8788e-03 at T = 1475.5878 K
147 !   max difference H/RT = 1.5898e-03 at T = 1654.2771 K
148 !   max difference S/R = 2.8144e-03 at T = 1738.9195 K
149 !   T_match = 1671.000000 jump
150 !   Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 0.000e+00, 7.105e-15)
151 !!HON      H      10      1N      1      OG      300.0000      5000.0000      1671.00      1
152 !! 3.78577430e+00 2.86062728e-03-1.02423922e-06 1.64463139e-10-9.77943616e-15      2
153 !! 2.93293258e+04 3.11911856e+00 3.39246137e+00 2.32348720e-03 1.27023231e-06      3
154 !!-1.66747061e-09 4.30367839e-13 2.95917808e+04 5.72341849e+00      4
155 ! Refitting species HONO:
156 !   max difference Cp/R = 3.2450e-06 at T = 986.5433 K
157 !   max difference H/RT = 1.6810e-06 at T = 1000.6503 K
158 !   max difference S/R = 5.1349e-06 at T = 1064.1321 K
159 !   T_match = 1000.000000 jump
160 !   Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 8.882e-16, 0.000e+00)
161 !!HONO      H      10      2N      1      OG      300.0000      5000.0000      1000.00      1
162 !! 5.48689300e+00 4.21806500e-03-1.64914300e-06 2.97187700e-10-2.02114800e-14      2
163 !!-1.12686517e+04-2.99700713e+00 2.29037472e+00 1.40995112e-02-1.36794846e-05      3
164 !! 7.49960538e-09-1.87721549e-12-1.04319463e+04 1.32809286e+01      4
165 ! Refitting species HONO2:
166 !   max difference Cp/R = 5.7786e-02 at T = 200.0000 K
167 !   max difference H/RT = 1.0515e-02 at T = 200.0000 K
168 !   max difference S/R = 9.3223e-03 at T = 200.0000 K
169 !   T_match = 1000.000000 jump
170 !   Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 3.553e-15,-7.105e-15)
171 !!HONO2      H      10      3N      1      OG      200.0000      6000.0000      1000.00      1
172 !! 8.03098942e+00 4.46958589e-03-1.72459491e-06 2.91556153e-10-1.80102702e-14      2
173 !!-1.92761511e+04-1.62575769e+01 1.03922026e+00 2.45362027e-02-2.45694284e-05      3
174 !! 1.37484493e-08-3.70491756e-12-1.73295877e+04 1.98317491e+01      4
175 ! Refitting species N:
176 !   max difference Cp/R = 3.6285e-04 at T = 899.5498 K
177 !   max difference H/RT = 5.9722e-05 at T = 1000.6503 K
178 !   max difference S/R = 9.1974e-05 at T = 1007.7039 K
179 !   T_match = 1000.000000 jump
180 !   Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 7.105e-15,-3.553e-15)
181 N      N      1      0      0      OG      300.0000      5000.0000      1000.00      1
182 2.45026800e+00 1.06614600e-04-7.46533700e-08 1.87965200e-11-1.02598400e-15      2
183 5.61159802e+04 4.44866603e+00 2.51239393e+00-9.42571483e-05 2.50330048e-07      3
184-2.77058774e-10 1.08591715e-13 5.60980027e+04 4.12910938e+00      4
185 ! Refitting species N2:
186 !   max difference Cp/R = 1.4577e-06 at T = 979.4897 K
187 !   max difference H/RT = 8.3069e-07 at T = 1000.6503 K
188 !   max difference S/R = 1.5396e-06 at T = 1024.1621 K
189 !   T_match = 1000.000000 jump
190 !   Delta(Cp/R, H/RT, S/R) = (-4.441e-16,-4.441e-16, 0.000e+00)
191 N2      N      2      0      0      OG      300.0000      5000.0000      1000.00      1
192 2.92664000e+00 1.48797680e-03-5.68476000e-07 1.00970380e-10-6.75335100e-15      2
193-9.22796869e+02 5.98052646e+00 3.29865872e+00 1.40837971e-03-3.96358857e-06      3
194 5.64191194e-09-2.44500396e-12-1.02089812e+03 3.95044772e+00      4
195 ! Refitting species N2H2:
196 !   max difference Cp/R = 4.5456e-08 at T = 999.6630 K
197 !   max difference H/RT = 5.2424e-08 at T = 1000.5143 K
198 !   max difference S/R = 7.9163e-09 at T = 1002.2170 K
199 !   T_match = 1000.000000 jump
200 !   Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, 0.000e+00, 0.000e+00)
201 N2H2      H      2N      2      0      OG      298.1500      2000.0000      1000.00      1
202 2.38388380e+00 6.63619559e-03-1.81669068e-06-1.19497031e-10 9.31659255e-14      2
203 2.34207531e+04 1.06091658e+01 4.14915912e+00-4.82013795e-03 2.19606590e-05      3
204-2.03662970e-08 6.25367446e-12 2.32874597e+04 3.19154082e+00      4
205 ! Refitting species N2H3:
206 !   max difference Cp/R = 5.6600e-02 at T = 200.0000 K
207 !   max difference H/RT = 1.0299e-02 at T = 200.0000 K
208 !   max difference S/R = 9.1309e-03 at T = 200.0000 K
209 !   T_match = 1000.000000 jump
210 !   Delta(Cp/R, H/RT, S/R) = (-3.553e-15, 0.000e+00, 0.000e+00)
211 N2H3      H      3N      2      0      OG      200.0000      6000.0000      1000.00      1
212 4.04483566e+00 7.31130186e-03-2.47625799e-06 3.83733021e-10-2.23107573e-14      2
213 2.48157541e+04 2.88824492e+00 2.78061414e+00 6.75511530e-03 6.36330365e-06      3
214-1.05699445e-08 3.91221319e-12 2.53630630e+04 1.04251784e+01      4
215 ! Refitting species N2H4:
216 !   max difference Cp/R = 9.3068e-02 at T = 200.0000 K
217 !   max difference H/RT = 1.6935e-02 at T = 200.0000 K

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218 ! max difference S/R = 1.5014e-02 at T = 200.0000 K
219 ! T_match = 1000.000000 jump
220 ! Delta(Cp/R, H/RT, S/R) = ( 3.553e-15, 0.000e+00, 0.000e+00)
221 N2H4 H 4N 2 0 OG 200.0000 6000.0000 1000.00 1
222 4.93957357e+00 8.75017187e-03 -2.99399058e-06 4.67278418e-10 -2.73068599e-14 2
223 9.29234679e+03 -2.68780235e+00 2.78129807e+00 8.24026776e-03 1.14042141e-05 3
224 -1.81663167e-08 6.87626313e-12 1.01838576e+04 1.00171442e+01 4
225 ! Refitting species N2O:
226 ! max difference Cp/R = 1.8296e-06 at T = 998.2991 K
227 ! max difference H/RT = 3.3682e-07 at T = 1000.6503 K
228 ! max difference S/R = 7.6205e-06 at T = 1000.6503 K
229 ! T_match = 1000.000000 jump
230 ! Delta(Cp/R, H/RT, S/R) = (-2.665e-15, 0.000e+00, 0.000e+00)
231 !!N2O O 1N 2 0 OG 300.0000 5000.0000 1000.00 1
232 !! 4.71897700e+00 2.87371400e-03 -1.19749600e-06 2.25055200e-10 -1.57533700e-14 2
233 !! 8.16581066e+03 -1.65724238e+00 2.54303878e+00 9.49233877e-03 -9.79315613e-06 3
234 !! 6.26425400e-09 -1.90197860e-12 8.76510188e+03 9.51130165e+00 4
235 ! Refitting species NH:
236 ! max difference Cp/R = 6.4973e-09 at T = 999.6630 K
237 ! max difference H/RT = 8.0635e-09 at T = 1000.5143 K
238 ! max difference S/R = 1.9533e-08 at T = 1000.5143 K
239 ! T_match = 1000.000000 jump
240 ! Delta(Cp/R, H/RT, S/R) = ( 4.441e-16, 0.000e+00, 0.000e+00)
241 NH H 1N 1 0 OG 298.1500 2000.0000 1000.00 1
242 3.38393047e+00 -3.04401048e-04 1.07871576e-06 -5.39749068e-10 8.56574985e-14 2
243 4.18557586e+04 2.60065698e+00 3.49138453e+00 2.48104619e-04 -1.22352540e-06 3
244 1.97740002e-09 -7.89210150e-13 4.17851517e+04 1.83667276e+00 4
245 ! Refitting species NH2:
246 ! max difference Cp/R = 1.4994e-08 at T = 999.6630 K
247 ! max difference H/RT = 3.1298e-08 at T = 1000.5143 K
248 ! max difference S/R = 5.9200e-08 at T = 1804.1893 K
249 ! T_match = 1000.000000 jump
250 ! Delta(Cp/R, H/RT, S/R) = ( 8.882e-16, -3.553e-15, 0.000e+00)
251 NH2 H 2N 1 0 OG 298.1500 2000.0000 1000.00 1
252 3.80751460e+00 1.74138848e-04 2.06281679e-06 -1.18308148e-09 2.00814234e-13 2
253 2.12757238e+04 1.57634401e+00 4.02590040e+00 -9.53250898e-04 4.13467075e-06 3
254 -2.81816337e-09 6.73046109e-13 2.12447390e+04 5.86220432e-01 4
255 ! Refitting species NH2OH:
256 ! max difference Cp/R = 4.6508e-02 at T = 200.0000 K
257 ! max difference H/RT = 8.4629e-03 at T = 200.0000 K
258 ! max difference S/R = 7.5029e-03 at T = 200.0000 K
259 ! T_match = 1000.000000 jump
260 ! Delta(Cp/R, H/RT, S/R) = ( 1.776e-15, -4.441e-16, 0.000e+00)
261 !!NH2OH H 3O 1N 1 OG 200.0000 6000.0000 1000.00 1
262 !! 3.88112502e+00 8.15708448e-03 -2.82615576e-06 4.37930933e-10 -2.52724604e-14 2
263 !! -6.85534125e+03 3.79485718e+00 2.68374332e+00 1.06389335e-02 -2.07348345e-06 3
264 !! -3.72343389e-09 2.09895275e-12 -6.53427866e+03 1.00639571e+01 4
265 ! Refitting species NH3:
266 ! max difference Cp/R = 7.1188e-06 at T = 998.2991 K
267 ! max difference H/RT = 8.8265e-07 at T = 998.2991 K
268 ! max difference S/R = 4.7840e-06 at T = 1470.8854 K
269 ! T_match = 1000.000000 jump
270 ! Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, -8.882e-16, 3.553e-15)
271 NH3 H 3N 1 0 OG 300.0000 5000.0000 1000.00 1
272 2.46190400e+00 6.05916600e-03 -2.00497700e-06 3.13600300e-10 -1.93831700e-14 2
273 -6.49327085e+03 7.47209222e+00 2.20428351e+00 1.01152784e-02 -1.46540008e-05 3
274 1.44737927e-08 -5.32904367e-12 -6.52548128e+03 8.12742204e+00 4
275 ! Refitting species NNH:
276 ! max difference Cp/R = 4.7918e-09 at T = 999.6630 K
277 ! max difference H/RT = 6.7231e-09 at T = 1000.5143 K
278 ! max difference S/R = 2.7707e-08 at T = 1000.5143 K
279 ! T_match = 1000.000000 jump
280 ! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 0.000e+00, 0.000e+00)
281 NNH H 1N 2 0 OG 298.1500 2000.0000 1000.00 1
282 2.78024159e+00 4.51114118e-03 -1.98147075e-06 3.61161241e-10 -1.55679242e-14 2
283 2.93473063e+04 9.91752872e+00 3.86231282e+00 -4.41898521e-04 6.38522097e-06 3
284 -5.84138799e-09 1.69125807e-12 2.91621298e+04 4.85334925e+00 4
285 ! Refitting species NO:
286 ! max difference Cp/R = 4.5309e-07 at T = 958.3292 K
287 ! max difference H/RT = 1.6767e-06 at T = 1000.6503 K
288 ! max difference S/R = 3.9887e-06 at T = 1661.3307 K
289 ! T_match = 1000.000000 jump
290 ! Delta(Cp/R, H/RT, S/R) = ( 0.000e+00, -1.776e-15, -3.553e-15)

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291 !!NO O 1N 1 0 OG 300.0000 5000.0000 1000.00 1
292 !! 3.24543500e+00 1.26913800e-03-5.01589000e-07 9.16928300e-11-6.27541900e-15 2
293 !! 9.80084168e+03 6.41729799e+00 3.37653523e+00 1.25311480e-03-3.30288819e-06 3
294 !! 5.21795989e-09-2.44632032e-12 9.81796166e+03 5.82961801e+00 4
295 ! Refitting species NO2:
296 ! max difference Cp/R = 1.0714e-06 at T = 972.4362 K
297 ! max difference H/RT = 4.5554e-07 at T = 1000.6503 K
298 ! max difference S/R = 1.9699e-06 at T = 1000.6503 K
299 ! T_match = 1000.000000 jump
300 ! Delta(Cp/R, H/RT, S/R) = ( 2.665e-15,-8.882e-16, 0.000e+00)
301 !!NO2 O 2N 1 0 OG 300.0000 5000.0000 1000.00 1
302 !! 4.68285900e+00 2.46242900e-03-1.04225900e-06 1.97690200e-10-1.39171700e-14 2
303 !! 2.26129246e+03 9.88596530e-01 2.67058570e+00 7.83861016e-03-8.06415290e-06 3
304 !! 6.16202774e-09-2.32026867e-12 2.89629239e+03 1.16121292e+01 4
305 ! Refitting species NO3:
306 ! max difference Cp/R = 8.8881e-02 at T = 200.0000 K
307 ! max difference H/RT = 1.6173e-02 at T = 200.0000 K
308 ! max difference S/R = 1.4339e-02 at T = 200.0000 K
309 ! T_match = 1000.000000 jump
310 ! Delta(Cp/R, H/RT, S/R) = ( 1.776e-15, 0.000e+00, 0.000e+00)
311 !!NO3 O 3N 1 0 OG 200.0000 6000.0000 1000.00 1
312 !! 7.48347702e+00 2.57772064e-03-1.00945831e-06 1.72314063e-10-1.07154008e-14 2
313 !! 6.13915999e+03-1.41555150e+01 1.16756871e+00 1.89796870e-02-1.40508671e-05 3
314 !! 2.31286562e-09 8.04083704e-13 7.90312364e+03 1.86747550e+01 4
315 ! Refitting species O:
316 ! max difference Cp/R = 5.2008e-03 at T = 200.0000 K
317 ! max difference H/RT = 9.4637e-04 at T = 200.0000 K
318 ! max difference S/R = 8.3902e-04 at T = 200.0000 K
319 ! T_match = 1000.000000 jump
320 ! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 0.000e+00,-3.553e-15)
321 !!O O 1 0 0 OG 200.0000 3500.0000 1000.00 1
322 !! 2.56942078e+00-8.59741137e-05 4.19484589e-08-1.00177799e-11 1.22833691e-15 2
323 !! 2.92181207e+04 4.78470723e+00 3.10939988e+00-2.78256310e-03 5.17445426e-06 3
324 !!-4.34517881e-09 1.36049345e-12 2.91275381e+04 2.29023724e+00 4
325 ! Refitting species O2:
326 ! max difference Cp/R = 6.2130e-03 at T = 200.0000 K
327 ! max difference H/RT = 1.1306e-03 at T = 200.0000 K
328 ! max difference S/R = 1.0023e-03 at T = 200.0000 K
329 ! T_match = 1000.000000 jump
330 ! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 0.000e+00,-3.553e-15)
331 !!O2 O 2 0 0 OG 200.0000 3500.0000 1000.00 1
332 !! 3.28253784e+00 1.48308754e-03-7.57966669e-07 2.09470555e-10-2.16717794e-14 2
333 !!-1.08781074e+03 5.45367161e+00 3.71213227e+00-2.40329876e-03 8.09286837e-06 3
334 !!-7.55141837e-09 2.34517397e-12-1.05763729e+03 3.94235871e+00 4
335 ! Refitting species OH:
336 ! max difference Cp/R = 3.0622e-03 at T = 200.0000 K
337 ! max difference H/RT = 5.5721e-04 at T = 200.0000 K
338 ! max difference S/R = 4.9400e-04 at T = 200.0000 K
339 ! T_match = 1000.000000 jump
340 ! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 0.000e+00, 0.000e+00)
341 !!OH H 1O 1 0 OG 200.0000 6000.0000 1000.00 1
342 !! 2.86472886e+00 1.05650448e-03-2.59082758e-07 3.05218674e-11-1.33195876e-15 2
343 !! 3.71917660e+03 5.70185771e+00 4.09064517e+00-2.93296453e-03 5.66294409e-06 3
344 !!-4.74879004e-09 1.61950580e-12 3.38464627e+03-5.50122048e-01 4
345 END
346 REACTIONS MOLES KELVINS
347
348 ! R0001
349 !!H+O2=O+OH 1.0400E+14 0.00000 7692.21
350 ! R0002
351 !!O+H2=H+OH 3.8180E+12 0.00000 3999.59
352 !!DUPLICATE
353 ! R0003
354 !!O+H2=H+OH 8.7920E+14 0.00000 9646.72
355 !!DUPLICATE
356 ! R0004
357 !!H2+OH=H2O+H 2.1600E+08 1.51000 1726.04
358 ! R0005
359 !!2OH=O+H2O 2.0000E+07 1.65100 317.53
360 !!DUPLICATE
361 ! R0006
362 !!2OH=O+H2O 2.6000E+11 -0.05700 -416.16
363 !!DUPLICATE

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364	! R0007			
365	H2+M=2H+M	4.5770E+19	-1.40000	52526.06
366	H2/2.5000/ H2O/12.0000/ AR/0.0000/ HE/0.0000/			
367	! R0008			
368	H2+AR=2H+AR	5.8400E+18	-1.10000	52526.06
369	! R0009			
370	H2+HE=2H+HE	5.8400E+18	-1.10000	52526.06
371	! R0010			
372	!!2O+M=O2+M	6.1650E+15	-0.50000	0.00
373	!!H2/2.5000/ H2O/12.0000/ AR/0.0000/ HE/0.0000/			
374	! R0011			
375	!!2O+AR=O2+AR	1.8860E+13	0.00000	-899.76
376	! R0012			
377	!!2O+HE=O2+HE	1.8860E+13	0.00000	-899.76
378	! R0013			
379	!!O+H+M=OH+M	4.7140E+18	-1.00000	0.00
380	!!H2/2.5000/ H2O/12.0000/ AR/0.7500/ HE/0.7500/			
381	! R0014			
382	!!H2O+M=H+OH+M	6.0640E+27	-3.32200	60783.89
383	!!H2/3.0000/ H2O/0.0000/ HE/1.1000/ N2/2.0000/ O2/1.5000/			
384	! R0015			
385	!!2H2O=H+OH+H2O	1.0060E+26	-2.44000	60476.93
386	! R0016			
387	!!H+O2 (+M)=HO2 (+M)	4.6508E+12	0.44000	0.00
388	!!LOW /	6.3660E+20	-1.72000	264.09/
389	!!TROE /	5.000E-01	1.00E-30	1.00E+30 /
390	!!H2/2.0000/ H2O/14.0000/ O2/0.7800/ AR/0.6700/ HE/0.8000/			
391	! R0017			
392	!!HO2+H=H2+O2	2.7500E+06	2.09000	-730.17
393	! R0018			
394	!!HO2+H=2OH	7.0790E+13	0.00000	148.45
395	! R0019			
396	!!HO2+O=O2+OH	2.8500E+10	1.00000	-364.30
397	! R0020			
398	!!HO2+OH=H2O+O2	1.9300E+20	-2.49000	293.88
399	!!DUPLICATE			
400	! R0021			
401	!!HO2+OH=H2O+O2	1.2100E+09	1.24000	-659.22
402	!!DUPLICATE			
403	! R0022			
404	!!2H+O2=H2+O2	8.8000E+22	-1.83500	402.58
405	! R0023			
406	!!2H+O2=2OH	4.0000E+22	-1.83500	402.58
407	! R0024			
408	!!H+O2+O=OH+O2	7.3500E+22	-1.83500	402.58
409	! R0025			
410	!!H+O2+OH=H2O+O2	2.5600E+22	-1.83500	402.58
411	! R0026			
412	!!2HO2=H2O2+O2	1.9300E-02	4.12000	-2495.97
413	! R0027			
414	!!2HO2=2OH+O2	6.4100E+17	-1.54000	4297.50
415	! R0028			
416	!!H2O2 (+M)=2OH (+M)	2.0000E+12	0.90000	24531.45
417	!!LOW /	2.4900E+24	-2.30000	24531.45/
418	!!TROE /	4.300E-01	1.00E-30	1.00E+30 /
419	!!H2O/7.5000/ N2/1.5000/ O2/1.2000/ HE/0.6500/ H2O2/7.7000/ H2/3.7000/			
420	! R0029			
421	!!H2O2+H=H2O+OH	2.4100E+13	0.00000	1997.78
422	! R0030			
423	!!H2O2+H=HO2+H2	4.8200E+13	0.00000	4000.60
424	! R0031			
425	!!H2O2+O=OH+HO2	9.5500E+06	2.00000	1997.78
426	! R0032			
427	!!H2O2+OH=HO2+H2O	1.7400E+12	0.00000	160.02
428	!!DUPLICATE			
429	! R0033			
430	!!H2O2+OH=HO2+H2O	7.5900E+13	0.00000	3658.41
431	!!DUPLICATE			
432	! R0034			
433	N2+M=2N+M	1.8900E+18	-0.85000	113224.40
434	!!H2O/16.2500/			
435	! R0035			
436	!!N+O+M=NO+M	7.6000E+14	-0.10000	-890.70

437	!!H2O/16.2500/			
438	! R0036			
439	!!N+NO2=N2O+O	1.8000E+12	0.00000	0.00
440	! R0037			
441	!!N+O2=NO+O	5.8410E+09	1.01000	3120.97
442	! R0038			
443	!!N+OH=NO+H	1.0840E+14	-0.20000	0.00
444	! R0039			
445	!!N+NO=N2+O	3.2000E+13	0.00000	0.00
446	! R0040			
447	NH+H=N+H2	1.6500E+11	0.71000	468.50
448	! R0041			
449	!!NH+O=NO+H	4.8200E+13	0.02300	47.81
450	! R0042			
451	!!NH+O=N+OH	2.0700E+10	0.62200	-180.15
452	! R0043			
453	!!NH+OH=HNO+H	3.2500E+14	-0.37600	-23.15
454	! R0044			
455	!!NH+OH=N+H2O	1.5900E+07	1.73300	-289.85
456	! R0045			
457	!!NH+O2=HNO+O	3.3200E+09	1.03400	5746.77
458	! R0046			
459	!!NH+O2=NO+OH	4.5000E+08	0.79000	601.35
460	! R0047			
461	2NH=>N2+H2	6.2600E+12	-0.03600	-80.97
462	! R0048			
463	2NH=>N2+2H	5.6340E+13	-0.03600	-80.97
464	! R0049			
465	NH+N=N2+H	3.0000E+13	0.00000	0.00
466	! R0050			
467	!!NH+NO=N2O+H	2.7000E+15	-0.78000	10.06
468	! R0051			
469	!!NH+NO=N2+OH	6.8000E+14	-0.78000	10.06
470	! R0052			
471	!!NH+NO2=N2O+OH	4.1000E+12	0.00000	0.00
472	! R0053			
473	!!NH+NO2=HNO+NO	5.9000E+12	0.00000	0.00
474	! R0054			
475	!!NH+HONO=NH2+NO2	1.0000E+13	0.00000	0.00
476	! R0055			
477	!!NH+N2O=N2+HNO	2.0000E+12	0.00000	3019.32
478	! R0056			
479	NH2+M=NH+H+M	1.2000E+15	0.00000	38246.07
480	! R0057			
481	NH2+H=NH+H2	1.0900E+05	2.59000	912.00
482	! R0058			
483	!!NH2+O=NH+OH	7.2300E+12	0.00000	0.00
484	! R0059			
485	!!NH2+O=HNO+H	1.5000E+15	-0.54700	421.04
486	!!DUPLICATE			
487	! R0060			
488	!!NH2+O=HNO+H	7.7300E+13	-0.27700	325.28
489	!!DUPLICATE			
490	! R0061			
491	!!NH2+OH=NH+H2O	4.0400E+04	2.52000	-310.00
492	! R0062			
493	!!NH2+HO2=H2NO+OH	5.0000E+13	0.00000	0.00
494	! R0063			
495	!!NH2+HO2=NH3+O2	2.1800E+06	2.08000	-2395.33
496	! R0064			
497	!!NH2+O2=H2NO+O	2.6000E+11	0.48720	14643.69
498	! R0065			
499	!!NH2+O2=HNO+OH	2.9000E-02	3.76400	9151.05
500	! R0066			
501	NH2+N=N2+2H	6.9000E+13	0.00000	0.00
502	! R0067			
503	!!NH2+NO=NNH+OH	3.1000E+13	-0.48000	593.80
504	! R0068			
505	!!NH2+NO=N2+H2O	1.1000E+20	-2.51400	644.12
506	! R0069			
507	!!NH2+NO2=H2NO+NO	8.6000E+11	0.11000	-596.82
508	! R0070			
509	!!NH2+NO2=N2O+H2O	2.2000E+11	0.11000	-596.82

510	! R0071			
511	!!NH2+HNO=NH3+NO	5.9000E+02	2.95000	-1745.67
512	! R0072			
513	!!NH2+HONO=NH3+NO2	4.8400E+00	3.36000	-2304.75
514	! R0073			
515	2NH=NH2+N	5.7000E-01	3.88000	172.10
516	! R0074			
517	2NH2=NH3+NH	5.6360E+00	3.53000	278.08
518	! R0075			
519	NH2+NH=NH3+N	9.5740E+03	2.46000	54.00
520	! R0076			
521	N2H2+M=NNH+H+M	1.9000E+27	-3.05000	33262.81
522	H2O/7.0000/			
523	! R0077			
524	N2H2+H=NNH+H2	4.8200E+08	1.76000	372.00
525	! R0078			
526	!!N2H2+O=NH2+NO	1.0000E+13	0.00000	0.00
527	! R0079			
528	!!N2H2+O=NNH+OH	1.1100E+08	1.62000	405.00
529	! R0080			
530	!!N2H2+OH=NNH+H2O	6.7400E+03	2.80000	-255.13
531	! R0081			
532	!!N2H2+NO=N2O+NH2	4.0000E+12	0.00000	5998.38
533	! R0082			
534	!!N2H2+NO2=NNH+HONO	1.2500E+00	3.80000	5233.48
535	! R0083			
536	N2H2+NH=NNH+NH2	2.4000E+06	2.00000	-599.84
537	! R0084			
538	N2H2+NH2=NNH+NH3	2.7100E+05	2.22600	-518.32
539	! R0085			
540	NH2+NH=N2H2+H	1.3000E+14	-0.27200	-38.75
541	! R0086			
542	2NH2=N2H2+H2	1.7000E+08	1.62000	5929.44
543	! R0087			
544	!!N2H2+HO2=NNH+H2O2	1.0000E+13	0.00000	999.90
545	! R0088			
546	2NH2 (+M)=N2H4 (+M)	5.6000E+14	-0.41400	33.21
547	LOW /	1.6000E+34	-5.49000	999.90/
548	TROE /	3.100E-01	1.00E-30	1.00E+30 1.00E+30/
549	AR/0.5900/ N2/1.0000/ O2/0.6900/ NH3/4.8700/			
550	! R0089			
551	N2H4=N2H2+H2	5.1900E+38	-7.84000	33766.03
552	! R0090			
553	N2H4+H=N2H3+H2	2.7600E+05	2.56000	613.93
554	! R0091			
555	!!N2H4+OH=N2H3+H2O	1.3000E+13	0.00000	-160.02
556	! R0092			
557	N2H4+NH2=N2H3+NH3	7.6000E-01	4.00000	2037.03
558	! R0093			
559	N2H4+N2H2=2N2H3	2.5000E+10	0.50000	14995.94
560	! R0094			
561	N2H4+NH=N2H3+NH2	1.0000E+12	0.00000	1001.41
562	! R0095			
563	!!N2H4+O=N2H2+H2O	4.4000E+11	0.00000	-639.09
564	! R0096			
565	!!N2H4+O=N2H3+OH	6.7000E+08	1.50000	1434.68
566	! R0097			
567	!!N2H4+NO=N2H3+HNO	6.0000E+01	3.16000	15521.81
568	! R0098			
569	!!N2H4+NO2=N2H3+HONO	8.2000E+01	3.13000	4458.53
570	! R0099			
571	!!N2H4+NO2=N2H3+HNO2	2.4000E-02	4.14000	3998.58
572	! R0100			
573	N2H3 (+M)=N2H2+H (+M)	1.2800E+11	0.81900	24204.86
574	LOW /	3.8400E+40	-6.88000	27425.47/
575	TROE /	8.420E-01	8.00E+04	2.80E+01 7.30E+03/
576	AR/1.0000/ N2/2.0000/			
577	! R0101			
578	N2H3+H=N2H2+H2	7.4760E+03	2.79600	2355.07
579	! R0102			
580	N2H3+H=H2NN+H2	6.2430E+06	1.89000	124.30
581	! R0103			
582	N2H3+H=NH3+NH	1.0000E+11	0.00000	0.00

583	! R0104			
584	!!N2H3+O=N2H2+OH	1.7000E+08	1.50000	-325.08
585	! R0105			
586	!!N2H3+O=NH2+HNO	3.0000E+13	0.00000	0.00
587	! R0106			
588	!!N2H3+O=>NH2+NO+H	3.0000E+13	0.00000	0.00
589	! R0107			
590	!!N2H3+OH=N2H2+H2O	1.2000E+06	2.00000	-599.84
591	! R0108			
592	!!N2H3+OH=H2NN+H2O	3.0000E+13	0.00000	0.00
593	! R0109			
594	!!N2H3+OH=NH3+HNO	1.0000E+12	0.00000	7548.29
595	! R0110			
596	!!N2H3+HO2=N2H2+H2O2	1.4000E+04	2.69000	-805.15
597	! R0111			
598	!!N2H3+HO2=N2H4+O2	9.2000E+05	1.94000	1069.84
599	! R0112			
600	N2H3+NH2=N2H2+NH3	6.0800E-01	3.57400	598.83
601	! R0113			
602	N2H3+NH2=H2NN+NH3	1.1100E+01	3.08000	106.18
603	! R0114			
604	N2H3+NH=N2H2+NH2	2.0000E+13	0.00000	0.00
605	! R0115			
606	N2H3+N2H2=N2H4+NNH	1.0000E+13	0.00000	5002.00
607	! R0116			
608	2N2H3=2NH3+N2	3.0000E+12	0.00000	0.00
609	! R0117			
610	2N2H2=N2H3+NNH	1.0000E+13	0.00000	4999.49
611	! R0118			
612	2NH2=H2NN+H2	7.2000E+04	1.88000	4429.34
613	! R0119			
614	H2NN=NNH+H	3.4000E+26	-4.83000	23258.81
615	! R0120			
616	H2NN+H=NNH+H2	4.8000E+08	1.50000	-449.88
617	! R0121			
618	H2NN+H=N2H2+H	7.0000E+13	0.00000	0.00
619	! R0122			
620	!!H2NN+O=NNH+OH	3.3000E+08	1.50000	-449.88
621	! R0123			
622	!!H2NN+O=NH2+NO	7.0000E+13	0.00000	0.00
623	! R0124			
624	!!H2NN+OH=NNH+H2O	2.4000E+06	2.00000	-599.84
625	! R0125			
626	!!H2NN+OH=>NH2+NO+H	2.0000E+12	0.00000	0.00
627	! R0126			
628	!!H2NN+HO2=>NH2+NO+OH	9.0000E+12	0.00000	0.00
629	! R0127			
630	!!H2NN+HO2=NNH+H2O2	2.9000E+04	2.69000	-805.15
631	! R0128			
632	!!H2NN+O2=NH2+NO2	1.5000E+12	0.00000	2999.69
633	! R0129			
634	H2NN+NH2=NNH+NH3	1.8000E+06	1.94000	-579.71
635	! R0130			
636	!!H2NO+M=HNOH+M	1.1000E+29	-4.00000	22141.66
637	!!H2O/10.0000/			
638	! R0131			
639	!!HNOH+M=HNO+H+M	2.0000E+24	-2.80000	29654.73
640	!!H2O/10.0000/			
641	! R0132			
642	!!HNOH+H=NH2+OH	4.0000E+13	0.00000	0.00
643	! R0133			
644	!!HNOH+H=HNO+H2	4.8000E+08	1.50000	190.22
645	! R0134			
646	!!HNOH+O=HNO+OH	7.0000E+13	0.00000	0.00
647	!!DUPLICATE			
648	! R0135			
649	!!HNOH+O=HNO+OH	3.3000E+08	1.50000	-180.15
650	!!DUPLICATE			
651	! R0136			
652	!!HNOH+OH=HNO+H2O	2.4000E+06	2.00000	-599.84
653	! R0137			
654	!!HNOH+HO2=HNO+H2O2	2.9000E+04	2.70000	-805.15
655	! R0138			

656	!!HNOH+O2=HNO+HO2	3.0000E+12	0.00000	12580.49	
657	! R0139				
658	!!HNOH+NH2=N2H3+OH	1.0000E+01	3.50000	-235.00	
659	! R0140				
660	!!HNOH+NH2=H2NN+H2O	8.8000E+16	-1.10000	560.08	
661	! R0141				
662	!!HNOH+NH2=NH3+HNO	1.8000E+06	1.90000	-579.71	
663	! R0142				
664	!!HNOH+NO2=HONO+HNO	6.0000E+11	0.00000	1006.44	
665	! R0143				
666	!!NH2OH (+M)=NH2+OH (+M)	1.4000E+20	-1.31000	32246.31	
667	!!LOW /	5.4000E+37	-5.96000	33605.00/	
668	!!TROE /	3.500E-01	1.00E-30	1.00E+30	1.00E+30/
669	! R0144				
670	!!NH2OH+H=HNOH+H2	4.8000E+08	1.50000	3144.62	
671	! R0145				
672	!!NH2OH+H=H2NO+H2	2.4000E+08	1.50000	2549.81	
673	! R0146				
674	!!NH2OH+O=HNOH+OH	3.3000E+08	1.50000	1944.94	
675	! R0147				
676	!!NH2OH+O=H2NO+OH	1.7000E+08	1.50000	1514.69	
677	! R0148				
678	!!NH2OH+OH=HNOH+H2O	1.5000E+04	2.61000	-1779.89	
679	! R0149				
680	!!NH2OH+OH=H2NO+H2O	1.5000E+05	2.28000	-652.17	
681	! R0150				
682	!!NH2OH+NH2=HNOH+NH3	1.1000E-01	4.00000	-48.81	
683	! R0151				
684	!!NH2OH+NH2=H2NO+NH3	9.5000E+00	3.42000	-509.76	
685	! R0152				
686	!!NH2OH+NH=HNOH+NH2	2.9000E-03	4.40000	787.04	
687	! R0153				
688	!!NH2OH+NH=H2NO+NH2	1.5000E-03	4.60000	1219.80	
689	! R0154				
690	!!NH2OH+HO2=HNOH+H2O2	2.9000E+04	2.69000	4809.27	
691	! R0155				
692	!!NH2OH+HO2=H2NO+H2O2	1.4000E+04	2.69000	3229.66	
693	! R0156				
694	!!HNOH+HNO=NH2OH+NO	1.0000E+12	0.00000	1509.66	
695	! R0157				
696	NH3+M=NH2+H+M	2.2000E+16	0.00000	47035.93	
697	! R0158				
698	NH3+H=NH2+H2	2.8900E+06	2.23000	5233.48	
699	! R0159				
700	!!NH3+OH=H2O+NH2	1.5590E+05	2.37200	59.83	
701	! R0160				
702	!!NH3+HO2=NH2+H2O2	1.1730E+00	3.83900	8685.57	
703	! R0161				
704	!!NH3+O=NH2+OH	4.4300E+02	3.18000	3391.65	
705	! R0162				
706	NH3+NH2=N2H3+H2	1.0000E+11	0.50000	10869.54	
707	! R0163				
708	NNH=N2+H	3.3000E+08	0.00000	0.00	
709	! R0164				
710	NNH+H=N2+H2	1.0000E+14	0.00000	0.00	
711	! R0165				
712	!!NNH+OH=N2+H2O	5.0000E+13	0.00000	0.00	
713	! R0166				
714	!!NNH+NO=N2+HNO	5.0000E+12	0.00000	0.00	
715	! R0167				
716	NNH+NH=N2+NH2	5.0000E+13	0.00000	0.00	
717	! R0168				
718	NNH+NH2=N2+NH3	5.0000E+13	0.00000	0.00	
719	! R0169				
720	!!NNH+O=N2O+H	1.8700E+14	-0.27400	-11.07	
721	! R0170				
722	!!NNH+O=NH+NO	5.1800E+11	0.38800	-205.82	
723	! R0171				
724	!!NNH+O=N2+OH	1.2000E+13	0.14500	-109.20	
725	! R0172				
726	!!NNH+O2=N2+HO2	5.6000E+14	-0.38500	-6.54	
727	! R0173				
728	2NNH=N2H2+N2	1.0000E+13	0.00000	4999.49	

729	! R0174					
730	!!HNO=H+NO			1.8259E+20	-3.00800	24094.15
731	!!PLOG/	0.1000	2.0121E+19	-3.0210	24049.8699/	
732	!!PLOG/	1.0000	1.8259E+20	-3.0080	24094.1532/	
733	!!PLOG/	10.0000	1.2762E+21	-2.9590	24204.8615/	
734	!!PLOG/	100.0000	5.6445E+21	-2.8550	24385.5173/	
735	!!PLOG/	1000.0000	9.7111E+21	-2.6420	24627.5659/	
736	! R0175					
737	!!HNO+O=NO+OH			2.3000E+13	0.00000	0.00
738	! R0176					
739	!!HNO+H=NO+H2			4.4000E+11	0.72000	327.09
740	! R0177					
741	!!HNO+OH=NO+H2O			3.6000E+13	0.00000	0.00
742	! R0178					
743	!!HNO+O2=NO+HO2			2.0000E+13	0.00000	8051.51
744	! R0179					
745	!!HNO+N=NO+NH			1.0000E+13	0.00000	1001.41
746	! R0180					
747	!!HNO+N=N2O+H			5.0000E+10	0.50000	1509.66
748	! R0181					
749	!!HNO+NH=NH2+NO			5.0000E+11	0.50000	0.00
750	! R0182					
751	!!HNO+NO=N2O+OH			8.5100E+12	0.00000	14900.33
752	! R0183					
753	!!HNO+NO2=HONO+NO			4.4000E+04	2.60000	2033.01
754	! R0184					
755	!!2HNO=N2O+H2O			9.0000E+08	0.00000	1559.98
756	! R0185					
757	!!HON+M=NO+H+M			5.1000E+19	-1.73000	8071.64
758	!!AR/0.7000/ H2O/7.0000/					
759	! R0186					
760	!!HON+H=HNO+H			2.4000E+13	0.00000	0.00
761	! R0187					
762	!!HON+H=OH+NH			1.0000E+13	0.00000	0.00
763	! R0188					
764	!!HON+O=OH+NO			7.0000E+13	0.00000	0.00
765	! R0189					
766	!!HON+OH=HONO+H			4.0000E+13	0.00000	0.00
767	! R0190					
768	!!HON+O2=NO2+OH			1.0000E+12	0.00000	2499.99
769	! R0191					
770	!!OH+NO=HONO			1.8000E+22	-3.10000	925.42
771	!!PLOG/	0.1000	6.9200E+21	-3.8600	293.1757/	
772	!!PLOG/	0.2154	1.4600E+22	-3.8500	356.3298/	
773	!!PLOG/	0.4641	2.9300E+22	-3.8400	427.8373/	
774	!!PLOG/	1.0000	5.3400E+22	-3.8200	505.7357/	
775	!!PLOG/	2.1540	8.5300E+22	-3.7800	588.2637/	
776	!!PLOG/	4.6410	1.1500E+23	-3.7200	674.3142/	
777	!!PLOG/	10.0000	1.2500E+23	-3.6300	759.8616/	
778	!!PLOG/	21.5400	1.0100E+23	-3.5000	837.3574/	
779	!!PLOG/	46.4100	5.4700E+22	-3.3300	896.7373/	
780	!!PLOG/	100.0000	1.8000E+22	-3.1000	925.4208/	
781	! R0192					
782	!!NO+HO2=NO2+OH			2.1000E+12	0.00000	-241.55
783	! R0193					
784	!!HONO+H=NO2+H2			1.9000E+03	2.80000	704.51
785	! R0194					
786	!!HNO2+H=NO2+H2			2.3000E+04	2.80000	-1006.44
787	! R0195					
788	!!NO2+H=NO+OH			1.3800E+13	0.29000	12.63
789	! R0196					
790	!!NO2+O=NO+O2			1.1000E+14	-0.50000	0.00
791	! R0197					
792	!!NO+O (+M)=NO2 (+M)			2.9500E+14	-0.40000	0.00
793	!!LOW /			3.3360E+20	-1.60000	0.00/
794	!!TROE /			8.000E-01	1.00E-30	1.00E+30
795	!!H2/1.0000/ H2O/6.4000/ O2/0.4500/ N2/0.4000/ AR/0.3500/ HE/0.3500/					1.00E+30/
796	! R0198					
797	!!NO2+OH (+M)=HONO2 (+M)			3.0000E+13	0.00000	0.00
798	!!LOW /			2.9380E+25	-3.00000	0.00/
799	!!TROE /			4.000E-01	1.00E-30	1.00E+30
800	! R0199					
801	!!2NO2=2NO+O2			4.5000E+12	0.00000	13888.86

802	! R0200				
803	!!NO2+HO2=HONO+O2		1.9100E+00	3.32000	1531.80
804	! R0201				
805	!!NO2+HO2=HNO2+O2		1.8500E+01	3.26000	2507.54
806	! R0202				
807	!!N2O(+M)=N2+O(+M)		1.3000E+12	0.00000	31486.45
808	!!LOW /		4.0000E+14	0.00000	28482.23/
809	!!N2/1.7000/ O2/1.4000/ H2O/12.0000/				
810	! R0203				
811	!!N2O+H=N2+OH		2.5300E+10	0.00000	2289.65
812	!!DUPLICATE				
813	! R0204				
814	!!N2O+H=N2+OH		5.0000E+14	0.00000	9108.27
815	!!DUPLICATE				
816	! R0205				
817	!!N2O+O=2NO		9.2000E+13	0.00000	13924.09
818	! R0206				
819	!!N2O+O=N2+O2		3.7000E+12	0.00000	8016.29
820	! R0207				
821	!!N2O+OH=N2+HO2		1.3000E-02	4.70000	18397.71
822	! R0208				
823	!!N2O+NO=NO2+N2		5.3000E+05	2.20000	23289.00
824	! R0209				
825	!!N2O+N=N2+NO		1.0000E+13	0.00000	9998.97
826	! R0210				
827	!!H2NO+M=HNO+H+M		2.8000E+24	-2.80000	32663.98
828	!!H2O/10.0000/				
829	! R0211				
830	!!H2NO+H=HNO+H2		4.8000E+08	1.50000	784.92
831	! R0212				
832	!!H2NO+H=NH2+OH		4.0000E+13	0.00000	0.00
833	! R0213				
834	!!H2NO+O=HNO+OH		3.3000E+08	1.50000	244.97
835	! R0214				
836	!!H2NO+OH=HNO+H2O		2.4000E+06	2.00000	599.94
837	! R0215				
838	!!H2NO+NH2=HNO+NH3		1.8000E+06	1.94000	-291.87
839	! R0216				
840	!!H2NO+HO2=HNO+H2O2		2.9000E+04	2.69000	-805.15
841	! R0217				
842	!!H2NO+O2=HNO+HO2		2.3000E+02	2.99400	8303.12
843	! R0218				
844	!!H2NO+NO=2HNO		2.0000E+04	2.00000	6541.85
845	! R0219				
846	!!H2NO+NO2=HONO+HNO		6.0000E+11	0.00000	1006.44
847	! R0220				
848	!!HONO+O=NO2+OH		1.2000E+13	0.00000	3019.32
849	! R0221				
850	!!HONO+H=HNO+OH		1.5000E+03	2.70000	2314.81
851	! R0222				
852	!!HONO+H=NO+H2O		4.3000E+09	1.00000	2063.20
853	! R0223				
854	!!HONO+OH=NO2+H2O		1.7000E+12	0.00000	-261.67
855	! R0224				
856	!!HONO+NO2=HONO2+NO		2.0000E+11	0.00000	16455.28
857	! R0225				
858	!!2HONO=NO+NO2+H2O		3.5000E-01	3.64000	6109.09
859	! R0226				
860	!!HNO2=HONO		2.6700E+20	-2.80000	21698.83
861	!!PLOG/ 0.1000	1.0900E+47	-11.4800	26237.8686/	
862	!!PLOG/ 0.2154	1.6000E+44	-10.6300	25553.4900/	
863	!!PLOG/ 0.4641	2.0100E+41	-9.7400	24889.2401/	
864	!!PLOG/ 1.0000	1.6500E+38	-8.7900	24235.0547/	
865	!!PLOG/ 2.1540	7.4900E+34	-7.7300	23590.9336/	
866	!!PLOG/ 4.6410	2.3200E+31	-6.6000	22987.0701/	
867	!!PLOG/ 10.0000	9.0500E+27	-5.4700	22473.7862/	
868	!!PLOG/ 21.5400	8.5300E+24	-4.4400	22081.2749/	
869	!!PLOG/ 46.4100	2.7300E+22	-3.5500	21829.6651/	
870	!!PLOG/ 100.0000	2.6700E+20	-2.8000	21698.8280/	
871	! R0227				
872	!!OH+NO=HNO2		1.0500E+09	0.25000	1485.00
873	!!PLOG/ 0.1000	1.9700E+18	-3.2900	1404.9890/	
874	!!PLOG/ 0.2154	2.6700E+17	-2.9300	1408.0084/	

875	!! PLOG/	0.4641	3.0900E+16	-2.5600	1404.4858/	
876	!! PLOG/	1.0000	3.1300E+15	-2.1700	1396.4343/	
877	!! PLOG/	2.1540	2.8600E+14	-1.7700	1387.3764/	
878	!! PLOG/	4.6410	2.4800E+13	-1.3700	1384.3570/	
879	!! PLOG/	10.0000	2.1200E+12	-0.9700	1392.4086/	
880	!! PLOG/	21.5400	1.8100E+11	-0.5700	1413.5438/	
881	!! PLOG/	46.4100	1.4800E+10	-0.1700	1446.7563/	
882	!! PLOG/	100.0000	1.0500E+09	0.2500	1485.0010/	
883	! R0228					
884	!! HNO2+H=NO+H2O			3.4000E+09	1.10000	2818.03
885	! R0229					
886	!! HNO2+H=HNO+OH			3.7000E+07	1.80000	2818.03
887	! R0230					
888	!! HNO2+O=NO2+OH			1.7000E+08	1.50000	1006.44
889	! R0231					
890	!! HNO2+OH=NO2+H2O			4.0000E+13	0.00000	0.00
891	! R0232					
892	!! HONO2+H=H2+NO3			5.6000E+08	1.50000	8252.80
893	! R0233					
894	!! HONO2+H=H2O+NO2			6.1000E+01	3.30000	3162.74
895	! R0234					
896	!! HONO2+H=OH+HONO			3.8000E+05	2.30000	3510.46
897	! R0235					
898	!! HONO2+OH=H2O+NO3			1.0000E+10	0.00000	-623.99
899	! R0236					
900	!! NO2+O(+M)=NO3(+M)			3.5000E+12	0.20000	0.00
901	!! LOW /			2.5000E+20	-1.50000	0.00/
902	!! TROE /			7.100E-01	1.00E-30	1.70E+03 1.00E+30/
903	! R0237					
904	!! 2NO2=NO3+NO			9.6000E+09	0.70000	10517.29
905	! R0238					
906	!! NO3+H=NO2+OH			6.0000E+13	0.00000	0.00
907	! R0239					
908	!! NO3+O=NO2+O2			1.0000E+13	0.00000	0.00
909	! R0240					
910	!! NO3+OH=NO2+HO2			1.4000E+13	0.00000	0.00
911	! R0241					
912	!! NO3+HO2=NO2+O2+OH			1.5000E+12	0.00000	0.00
913	! R0242					
914	!! NO3+NO2=NO+NO2+O2			5.0000E+10	0.00000	1479.47
915	! R0243					
916	!! 2NO3=2NO2+O2			5.1200E+11	0.00000	2450.68
917	END					
918						